Wednesday 19 February 2020 – at 11.00 a.m.
Seminar Room “-1” – Department of Mathematics

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From Crystals to Polycrystals

Abstract:
In this talk we discuss the emergence of an energy defined on rigid polycrystalline materials from atomistic systems with the Heitmann-Radin Sticky disc energy. The discrete energy is a suitably rescaled pair interaction energy, where the interaction potential models the atoms as hard spheres, that is minimized, when the two spheres, modelling the atoms, are tangential. Furthermore, the discrete energy is frame invariant and no underlying reference frame on the atomistic configurations is assumed. The continuum parameter is a piecewise constant function, that describes the local orientation and micro-translation of the configuration. The limit energy, derived by means of Gamma-convergence, is local and concentrated on the grain boundaries, i.e. on the boundaries of the zones where the underlying microscopic configuration has constant orientation. The surface energy density depends on the relative orientation of the two grains, their microscopic translation misfit, and the normal to the interface. We point out the differences of the derived continuum energy density with respect to the Read-Shockley formula. This is joint work with Manuel Friedrich and Bernd Schmidt.

Contact person: Gian Paolo Leonardi

The speaker is guest as part of the Research in Pairs program